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The Crystallography of Coxeter Groups

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INTRODUCTION

This paper is primarily concerned with the structure of those space groups in n-dimensional Euclidean space for which the point groups are generated by reflections, i.e., are crystallographic Coxeter groups. The determination of *all* possible space groups dates back to the last century for $n \leqslant 3$ and has recently been extended to $n = 4$ by Brown, Neubüser and Zassenhaus [3–5] with the aid of a computer and some previous work by Dade [7]. However, since eventually every finite group will occur as the point group of some space group, one cannot expect a reasonable solution to the problem for a general n. On the other hand, by restricting oneself to an accessible class of point groups, such as we have chosen, one can hope to obtain a satisfactory answer. The interest in Coxeter point groups is also heightened by the fact that, together with their subgroups, such groups are sufficient for $n \leqslant 3$. Our discussion can thus form the basis of a less *ad hoc* exposition than the one usually employed in that case [6]. A sequel [11] dealing with the systematic treatment of the case when the point group is the rotation subgroup of a Coxeter group will appear soon.

In Section 1, we present a general discussion of the problems of mathematical crystallography in affine space, including in particular a generalization of some results of Zassenhaus [10]. This is extended in Section 2 in the special case of Euclidean space. The principal results are presented in Section 3 and then applied in Section 4 to the classical situation. We also include an interpretation in our terms of the maximal groups found by Dade [7] in the case $n = 4$ and Ryškov [9] in the case $n = 5$.

After this was written, a paper of Schwarzenberger [12] appeared containing, among other things, some further results in the special case $C_1 \times \cdots \times C_1$.

1. Space Groups in Affine Space

Let E be a finite dimensional real affine space, V its vector space of translations and $A(E)$ the affine group of E. After choosing an origin, elements of $A(E)$ can be written in the form (t, g), where $t \in V$ and $g \in GL(V)$. They compose according to the rule $(t, g)(t', g') = (t + gt', gg')$; the inverse of (t, g) is $(-g^{-1}t, g^{-1})$.

A subgroup S of $A(E)$ is called a *space group* if $\Lambda = S \cap V$ is a lattice in V. The projection of S on $GL(V)$ is called the *point group* K of S. Elements of K leave Λ invariant, for if (a, g) is a representative in S of $g \in K$ and $t \in \Lambda$, the element $(a, g)(t, 1)(a, g)^{-1} = (gt, 1) \in S$ and therefore $gt \in \Lambda$. We can thus regard Λ as a K-module and S as an extension of Λ by K.

Suppose $\{(s(x), x)\}$ is a system of representatives in S of elements $x \in K$. The function $s\colon K \to V$ is not unique. However, if $\{(s'(x), x)\}$ is another such system, then $(s(x), x)(s'(x), x)^{-1} = (s(x) - s'(x), 1) \in \Lambda$ for all $x \in K$ so that the function $\bar{s}\colon K \to V/\Lambda$ obtained from s by reducing its values mod Λ *is* uniquely determined by S. Since

$$(s(x), x)(s(y), y) = (s(x) + xs(y) - s(xy), 1)(s(xy), xy),$$

the cohomology class of S in $H^2(K, \Lambda)$ is described by the cocycle $f(x, y) = s(x) + xs(y) - s(xy)$. As the values of f lie in Λ, $\bar{s}$ has the property $\bar{s}(xy) = \bar{s}(x) + x\bar{s}(y)$, i.e., it is a cocycle. Conversely, given a cocycle $K \to V/\Lambda$, we can lift its values in some fashion to V, obtaining a function $s\colon K \to V$. The set of elements in $A(E)$ of the form $(t + s(x), x)$, where $t \in \Lambda$ and $x \in K$, is then a space group with lattice Λ and point group K, which induces the given cocycle by the previous construction. The exact sequence $0 \to \Lambda \to V \to V/\Lambda \to 0$ gives rise to the long exact sequence

$$\cdots \longrightarrow H^1(K, V) \longrightarrow H^1(K, V/\Lambda) \xrightarrow{\delta} H^2(K, \Lambda) \longrightarrow H^2(K, V) \longrightarrow \cdots \tag{1}$$

and the definition of δ shows that $\delta\{\bar{s}\} = \{f\}$. In particular, if $H^2(K, V) = 0$, every extension of Λ by K is isomorphic to a space group. When K is finite, this is true and was already noticed by Zassenhaus [10].

Suppose a space group S' is conjugate to S by a translation $(a, 1)$. Then every element in S' is of the form $(a, 1)(t, x)(a, 1)^{-1} = (t + a - xa, x)$, where $(t, x) \in S$. It follows that S' has the same lattice and point group as S but that its cocycle $\bar{s}'$ differs from $\bar{s}$ by the coboundary $x \to \bar{a} - x\bar{a}$. In other words, S' and S define the same cohomology class in $H^1(K, V/\Lambda)$; the converse is clear. Secondly, it is easy to see that S' will be conjugate to S by an element of the form $(0, g)$ if and only if

$$\Lambda' = g\Lambda, \qquad K' = gKg^{-1}, \qquad \bar{s}'(x) = g\bar{s}(g^{-1}xg). \tag{2}$$

The conjugacy classes of space groups in $A(E)$ can therefore be determined as follows. Call a subgroup K of $GL(V)$ *crystallographic* if it leaves a lattice invariant and find the conjugacy classes of such subgroups in $GL(V)$. For each class $\{K\}$, consider the set $L(K)$ of lattices left invariant by K. The normaliser $N(K)$ of K in $GL(V)$ acts naturally on $L(K)$. For each orbit $\{\Lambda\}$ in $L(K)$ under this action, calculate the cohomology group $H^1(K, V/\Lambda)$. Let $N(K, \Lambda)$ be the intersection of $N(K)$ with $GL(\Lambda)$ and define an action of $N(K, \Lambda)$ on $H^1(K, V/\Lambda)$ by

$$\bar{s}^g(x) = g\bar{s}(g^{-1}xg), \tag{3}$$

in accordance with (2). The orbits of $H^1(K, V/\Lambda)$ then correspond to non-conjugate space groups with lattice Λ and point group K. Since elements of K leave invariant the lattices in $L(K)$, it suffices to consider the induced action of $\bar{N}(K) = N(K)/K$ on $L(K)$. Similarly, if $g \in K$, $\bar{s}^g(x) = \bar{s}(x) + x\bar{s}(g) - \bar{s}(g)$, which means that the action of K on $H^1(K, V/\Lambda)$ is trivial and one is reduced to considering the action of $\bar{N}(K, \Lambda) = N(K, \Lambda)/K$.

To calculate $H^1(K, V/\Lambda)$, one can employ the following method of Zassenhaus [10]. Choose a presentation F/R of K; let $\{e_i\}_{i\in I}$ be the generators and $\{R_j\}_{j\in J}$ the relations. By first reducing elements of F modulo R, one obtains an action of F on V. A cocycle $c: F \to V$ is uniquely determined by the vector $\mathbf{c} = (c(e_i))$, which may be prescribed arbitrarily. Furthermore, the restriction of c to R is determined by the set of values $(c(R_j))$ since, for $u \in F$, we have $c(uR_ju^{-1}) = uc(R_j) + c(u) - uR_ju^{-1}c(u) = uc(R_j)$ because uR_ju^{-1}, being in R, acts trivially on V. Using the cocycle property of c, we can express $c(R_j)$ as $\sum_i R_{ji}c(e_i)$ for certain $R_{ji} \in \mathbb{Z}[K]$, the integral group ring of K. Let $\mathbf{R}$ be the $J \times I$ matrix (R_{ji}); multiplication by $\mathbf{R}$ induces a linear mapping $V^I \to V^J$. Let M be the quotient group $\mathbf{R}^{-1}(\Lambda^J)/\mathbf{R}^{-1}\mathbf{R}(\Lambda^I)$.

Given $g \in N(K, \Lambda)$, choose a system of representatives $x_i \in F$ of elements $g^{-1}e_ig \in K$. Suppose that, for $\mathbf{c} \in R^{-1}(\Lambda^J)$, we define $c^g(e_i)$ to be $gc(x_i)$. If $\{y_i\}$ is another choice of representatives, $x_i^{-1}y_i \in R$ and $gc(y_i) = gc(x_ix_i^{-1}y_i) = gc(x_i) + gx_ic(x_i^{-1}y_i)$, which shows that the two possible definitions of $\mathbf{c}^g$ differ by an element of $\Lambda^I \subset \mathbf{R}^{-1}\mathbf{R}(\Lambda^I)$. One obtains therefore an action of $N(K, \Lambda)$ on M. If we express $c(x_i)$ as $\sum_k X_{ik}c(e_k)$, for some $X_{ik} \in \mathbb{Z}[K]$, the action of $g \in N(K, \Lambda)$ amounts to multiplication by the $I \times I$ matrix $\mathbf{X}(g) = (gX_{ik})$.

PROPOSITION 1.1. *Suppose $H^1(K, V) = 0$. Then $H^1(K, V/\Lambda)$ is isomorphic to M as $N(K, \Lambda)$-modules.*

Proof. Starting from $\mathbf{c} \in \mathbf{R}^{-1}(\Lambda^J)$, one obtains a cocycle $c: F \to V$ and then, by reducing its values mod Λ, a cocycle $F \to V/\Lambda$. Since $\mathbf{Rc} = (c(R_j))$ is in Λ^J, the latter cocycle vanishes on R and consequently induces a cocycle $\bar{c}: K \to V/\Lambda$. Let $\{\bar{c}\}$ be the cohomology class of $\bar{c}$ in $H^1(K, V/\Lambda)$.

We shall use the following exact sequences of cohomology groups:

$$0 \longrightarrow H^1(K, V/\Lambda) \xrightarrow{\text{inf}} H^1(F, V/\Lambda) \tag{4a}$$

$$H^1(F, \Lambda) \xrightarrow{\beta} H^1(F, V) \longrightarrow H^1(F, V/\Lambda) \longrightarrow 0 \tag{4b}$$

$$0 \longrightarrow H^1(K, V) \xrightarrow{\text{inf}} H^1(F, V) \xrightarrow{\text{res}} H^1(R, V); \tag{4c}$$

the zero on the right side of (4b) appears because $H^2(F, V) = 0$, F being a free group.

If $\{\bar{c}\} = 0$, the cohomology class of c in $H^1(F, V)$ lies in the image of β by (4b), so that $c(x) = d(x) + b - xb$ for some $b \in V$ and a cocycle $d: F \to \Lambda$, determined by the vector $\mathbf{d} = (d(e_i)) \in \Lambda^I$. Therefore $c(R_j) = d(R_j)$ or $\mathbf{Rc} = \mathbf{Rd}$, which means that $\mathbf{c} \in \mathbf{R}^{-1}\mathbf{R}(\Lambda^I)$. Conversely, if this condition is satisfied and $H^1(K, V) = 0$, the exact sequence (4c) shows that c and d belong to the same cohomology class in $H^1(F, V)$. Since the class of d lies in the image of β, $\{c\} = 0$ in $H^1(F, V/\Lambda)$ which implies, in view of (4a), that $\{\bar{c}\} = 0$ in $H^1(K, V/\Lambda)$.

It follows that the map $\mathbf{c} \to \{\bar{c}\}$ induces an injective homomorphism $M \to H^1(K, V/\Lambda)$. To see that it is also surjective, note that the exactness of (4b) implies that a cohomology class $\{\xi\} \in H^1(K, V/\Lambda)$, regarded as an element of $H^1(F, V/\Lambda)$ by (4a), is the image of some class $\{c\} \in H^1(F, V)$. Suppose $\xi(x) = \overline{c(x)} + \bar{a} - x\bar{a}$ for some $\bar{a} \in V/\Lambda$; then $0 = \xi(R_j) = \overline{c(R_j)}$, so that $\mathbf{Rc} = (c(R_j))$ belongs to Λ^J.

Finally, note that the element $\mathbf{c}^g = (gc(x_i))$, for $g \in N(K, \Lambda)$, is mapped to the cocycle $K \to V/\Lambda$ whose values on the generators $\bar{e}_i$ of K coincide with those of $\bar{c}^g$ as defined by (3) and which are consequently equal.

Suppose that K is finitely presented. Having chosen a basis for Λ, one can represent elements of $\mathbb{Z}[K]$ as $n \times n$ integral matrices, where $n = \dim(V)$. The matrix $\mathbf{R}$ becomes an $nJ \times nI$ integral matrix and each matrix $\mathbf{X}(g)$ an $nI \times nI$ integral matrix. Let $\mathbf{\Delta} = \mathbf{PRQ}$ be the Smith normal form of $\mathbf{R}$, where $\mathbf{\Delta} = \operatorname{diag}\{d_1, ..., d_r, 0, ..., 0\}$, $d_i > 0$ and $d_1 \mid \cdots \mid d_r$. The mapping $\mathbf{c} \to \mathbf{Q}^{-1}\mathbf{c}$ induces an isomorphism from M to $\mathbf{\Delta}^{-1}(\mathbb{Z}^{nJ})/\mathbf{\Delta}^{-1}\mathbf{\Delta}(\mathbb{Z}^{nI})$, which in turn is clearly isomorphic to $\mathbb{Z}/d_1\mathbb{Z} \oplus \cdots \oplus \mathbb{Z}/d_r\mathbb{Z}$. Thus, under the assumption of the theorem,

$$H^1(K, V/\Lambda) \simeq \mathbb{Z}/d_1\mathbb{Z} \oplus \cdots \oplus \mathbb{Z}/d_r\mathbb{Z}, \tag{5}$$

where the action of $g \in N(K, \Lambda)$ on the right side is multiplication by the principal $r \times r$ submatrix of $\mathbf{Q}^{-1}\mathbf{X}(g)\mathbf{Q}$. In particular, $H^1(K, V/\Lambda)$ is finite.

A substantial part of $H^1(K, V/\Lambda)$ can be obtained as follows. If Λ is a lattice invariant under K, we define the *weight group* of Λ to be the subgroup Λ^* of V consisting of all $x \in V$ such that $x - gx \in \Lambda$ for all $g \in K$. Clearly $\Lambda^* \supset \Lambda$ and $\Lambda^*/\Lambda = (V/\Lambda)^K$; the group $N(K, \Lambda)$ acts naturally on Λ^*/Λ.

When $V^K = 0$ and $H^1(K, V) = 0$, the exact sequence (1) shows that $\Lambda^*/\Lambda \cong H^1(K, \Lambda)$. In particular, if K is finite and $V^K = 0$, then Λ^*/Λ is also finite and Λ^* is therefore a lattice. A cocycle $\bar{t}\colon K \to V/\Lambda$ whose values lie in Λ^*/Λ will be called *weightlike*; it is then simply a homomorphism from K to Λ^*/Λ. The exact sequence $0 \to \Lambda^*/\Lambda \to V/\Lambda \to V/\Lambda^* \to 0$ gives rise to the long exact sequence

$$0 \longrightarrow \Lambda^{**}/\Lambda^* \longrightarrow \mathrm{Hom}(K, \Lambda^*/\Lambda) \xrightarrow{\gamma} H^1(K, V/\Lambda) \longrightarrow \cdots; \qquad (6)$$

the image of γ will be called the group of *weightlike classes* and denoted by $\Omega(K, \Lambda)$; it is invariant under the action of $N(K, \Lambda)$.

We consider next the effect of adding the inversion -1 to the point group K. Suppose $-1 \notin K$; we denote by $\pm K$ the subgroup generated by K and -1. It is clear that the same lattices are left invariant by both K and $\pm K$ and that $N(K) \subset N(\pm K)$. However, it may happen that inequivalent lattices for K may be equivalent for $\pm K$.

PROPOSITION 1.2. *If Λ is a lattice invariant under K, then $H^1(\pm K, V/\Lambda)$ is isomorphic to the direct sum of the group of elements of order $\leqslant 2$ in $H^1(K, V/\Lambda)$ and the quotient of Λ^*/Λ by $2(\Lambda^*/\Lambda)$.*

Proof. Regarding $\{\pm 1\}$ as the quotient of $\pm K$ by K, we have the exact sequence

$$0 \longrightarrow H^1(\{\pm 1\}, (V/\Lambda)^K) \xrightarrow{\text{inf}} H^1(\pm K, V/\Lambda) \xrightarrow{\text{res}} H^1(K, V/\Lambda)^{\{\pm 1\}}.$$

The group on the right consists of elements of order $\leqslant 2$ in $H^1(K, V/\Lambda)$ while that on the left is isomorphic to the quotient of Λ^*/Λ by $2(\Lambda^*/\Lambda)$. The homomorphism res is surjective in this case since a cocycle $t\colon K \to V/\Lambda$ such that $2t(g) = \bar{a} - g\bar{a}$ for some $\bar{a} \in V/\Lambda$ and all $g \in K$ can be extended to a cocycle $\pm K \to V/\Lambda$ by defining $t(-g) = \bar{a} - t(g)$. As all groups in the sequence are annihilated by 2, the sequence splits.

Finally, we note the following fact, first observed by Bieberbach [1] when K is finite.

PROPOSITION 1.3. *Suppose S is a space group with lattice Λ and point group K such that* (i) *K has no elements of the form $1 + n$, where $n^2 = 0$ but $n \neq 0$ and* (ii) *$H^1(K, V) = 0$. If S' is a space group isomorphic to S, then S' is conjugate to S in $A(E)$.*

Proof. It is easy to see that Λ is a normal and maximal abelian subgroup of S. Using assumption (i), we can show that these properties characterize Λ. For suppose A was another such subgroup; then A would contain an element (a, g) with $g \neq 1$. Being normal in S, it would contain the commutator

$[(t, 1), (a, g)] = ((1 - g)t, 1)$ for all $t \in \Lambda$. Being abelian, the commutator $[((1 - g)t, 1), (a, g)] = ((1 - g)^2 t, 1)$ must be trivial, i.e., $(1 - g)^2 = 0$ and so $g = 1$, a contradiction.

It follows that an isomorphism $\psi: S \to S'$ must map Λ onto Λ'. As a mapping $\Lambda \to \Lambda'$, ψ can be extended by linearity to an element $g \in GL(V)$. Replacing S' by the conjugate subgroup $(0, g)^{-1} S'(0, g)$ allows us to assume that $\Lambda' = \Lambda$ and that ψ is the identity on Λ. Consider an element $(t, x) \in S$ and suppose that $\psi(t, x) = (t', x')$. For every $a \in \Lambda$, applying ψ to the identity $(t, x)(a, 1)(t, x)^{-1} = (xa, 1)$, we conclude that $x'a = xa$, i.e., $x' = x$. This means that $K' = K$ and ψ induces the identity on K. In other words, ψ is an isomorphism between S and S' considered as extensions of Λ by K and therefore both S and S' correspond to the same cohomology class in $H^2(K, \Lambda)$. If $H^1(K, V) = 0$, the homomorphism δ in the exact sequence (1) is injective. This implies that the cocycles defined by S and S' belong to the same cohomology class in $H^1(K, V/\Lambda)$, i.e., that S' is conjugate to S by a translation.

One can show that assumption (i) necessarily holds if the elements of K leave invariant a nondegenerate symmetric bilinear form (x, y) of index one. This fact has also been noted by Janner and Ascher [8]. Indeed, we have $((1 + n)x, y) = (x, (1 - n)y)$ or $(nx, y) + (x, ny) = 0$ for all $x, y \in V$. In particular, (nx, x) and (nx, nx) are zero. If x is isotropic, this means that nx must be a multiple of x, since otherwise x and nx would span a two-dimensional totally isotropic subspace of V. It follows that $nx = 0$ and, since V has a basis of isotropic vectors, that $n = 0$.

2. Euclidean Space Groups

Let (x, y) be a positive definite nondegenerate symmetric bilinear form and Γ its orthogonal group.

PROPOSITION 2.1. (a) *Subgroups K and K' of Γ are conjugate in $GL(V)$ if and only if they are conjugate in Γ.*

(b) *The normalizer of a subgroup K of Γ in $GL(V)$ equals $C(K)\, N_\Gamma(K)$, where $C(K)$ is the centralizer of K in $GL(V)$ and $N_\Gamma(K)$ the normalizer of K in Γ.*

Proof. Suppose $K' = sKs^{-1}$ for some $s \in GL(V)$ and let $s = pu$ be the polar decomposition of s, with p hermitian and $u \in \Gamma$. Since $p^{-1}K'p = uKu^{-1} \in \Gamma$, the elements of $p^{-1}K'p$ satisfy $(p^{-1}xp)^*(p^{-1}xp) = 1$ or $xp^2 = p^2x$ for all $x \in K'$ (here $*$ denotes the adjoint involution). Since x and p^2 are normal and commute, they are simultaneously diagonalizable over $\mathbb{C}$. As p is the positive hermitian square root of p^2, it is also diagonal relative to such a basis and therefore commutes with x. Thus $p^{-1}K'p = K'$ and $K' = uKu^{-1}$, proving (a). Taking $K' = K$ in the argument, we conclude that $p \in C(K)$ and $u \in N_\Gamma(K)$, which proves (b).

Suppose K is a subgroup of Γ; let V^K be the subspace of elements fixed by K and V_K the orthogonal complement of V^K in V; both V^K and V_K are invariant under K. If $V^K = 0$, K is called *essential*; in general, the restriction $\bar{K}$ of K to V_K is essential. One sees easily that subgroups K and K' of Γ are conjugate in Γ iff there exists an isometry v: $V_K \to V_{K'}$ such that $v\bar{K}v^{-1} = \bar{K}'$. Furthermore, we have

$$N(K) = GL(V^K) \times N(\bar{K}) \tag{7}$$

since both V^K and V_K are invariant under $N(K)$, V_K being the sum of all irreducible nontrivial K-submodules of V.

The form (x, y) induces a metric space structure on the affine space E. A space group S will consist of isometries wrt this structure iff its point group K is contained in Γ (and is therefore finite). We assume from now on that this is the case.

Suppose Λ is a lattice invariant under K. Let $\Lambda^K = \Lambda \cap V^K$, $\Lambda_K = \Lambda \cap V_K$ and $\Lambda_0 = \Lambda^K \oplus \Lambda_K$. If $x = y + z \in \Lambda$, where $y \in V^K$ and $z \in V_K$, then $x - gx = z - gz \in \Lambda_K$, so that $z \in \Lambda_K{}^*$. The mapping $x \to z$ induces a homomorphism $\Lambda/\Lambda_0 \to \Lambda_K{}^*/\Lambda_K$ which is injective since if $z \in \Lambda_K$, $y = x - z \in \Lambda^K$ and thus $x \in \Lambda_0$. It follows that Λ/Λ_0 is finite and Λ_0 is a lattice. Let $\Theta(\Lambda)$ be the image of Λ/Λ_0 in $\Lambda_K{}^*/\Lambda_K$. The mapping $x \to y$ also induces an injective homomorphism $\Lambda/\Lambda_0 \to V^K/\Lambda^K$ whose image is isomorphic to $\Theta(\Lambda)$. Conversely, given lattices $\Lambda^K \subset V^K$ and $\Lambda_K \subset V_K$ and a subgroup Θ of $\Lambda_K{}^*/\Lambda_K$ which is isomorphic to a subgroup Θ_1 of V^K/Λ^K, one can construct a lattice $\Lambda \supset \Lambda_0 = \Lambda^K \oplus \Lambda_K$ such that $\Theta(\Lambda) = \Theta$. Namely, let κ: $\Theta \to \Theta_1$ be some isomorphism and define

$$\Lambda = \bigcup_{\theta \in \Theta} (y_{\kappa(\theta)} + z_\theta + \Lambda_0), \tag{8}$$

where z_θ (resp. $y_{\kappa(\theta)}$) are representatives of the elements of Θ (resp. Θ_1) in V_K (resp. V^K).

PROPOSITION 2.2. *If Λ and Λ' are lattices invariant under K, then $\Lambda' = s\Lambda$ for some $s \in N(K)$ iff there exists $t \in N(\bar{K})$ which maps Λ_K to $\Lambda_K{}'$ and induces an isomorphism $\Theta(\Lambda) \to \Theta(\Lambda')$.*

Proof. The necessity of the conditions is clear from Eq. (7). Conversely, let Θ_1 and $\Theta_1{}'$ be the isomorphic images of Λ/Λ_0 and $\Lambda'/\Lambda_0{}'$ in V^K/Λ^K and V^K/Λ'^K. We claim the existence of some $r \in GL(V^K)$ which maps Λ^K to Λ'^K and induces an isomorphism $\Theta_1 \to \Theta_1{}'$. To see this, let M^K (resp. M'^K) be the inverse images in V^K of Θ_1 (resp. $\Theta_1{}'$). By the invariant factor theorem, there exist integers $m_1, \ldots, m_k$ such that $m_1 \mid \cdots \mid m_k$ and bases $\{v_1, \ldots, v_k\}$ of Λ^K and $\{w_1, \ldots, w_k\}$ of Λ'^K such that $\{v_1/m_1, \ldots, v_k/m_k\}$ and $\{w_1/m_1, \ldots, w_k/m_k\}$ are bases of M^K and M'^K. It suffices to define r by $r(v_i) = w_i$ for $1 \leqslant i \leqslant k$. Using (8), it is clear that $s = (r, t)$, which belongs to $N(K)$, will map Λ to Λ'.

It follows that in order to obtain a representative set of lattices invariant under K, one should first choose a representative set of lattices $\Lambda_K \subset V_K$ invariant under $\bar{K}$ and an arbitrary lattice $\Lambda^K \subset V^K$. For each Λ_K, one then chooses a representative set of subgroups Θ of $\Lambda_K{}^*/\Lambda_K$ from those which are isomorphic to subgroups of V^K/Λ^K. Finally, one combines Λ_K, Λ^K and Θ by (8).

Unfortunately, we have not been able to obtain a formula for $H^1(K, V/\Lambda)$ in terms of these ingredients. In the special case when $\Lambda = \Lambda_0$, we have

$$H^1(K, V/\Lambda_0) \simeq H^1(\bar{K}, V_K/\Lambda_K) \oplus \operatorname{Hom}(K, V^K/\Lambda^K). \tag{9}$$

In general, the exact sequence $0 \to \Lambda/\Lambda_0 \to V/\Lambda_0 \to V/\Lambda \to 0$ gives rise to the long exact sequence

$$\cdots \longrightarrow (V/\Lambda_0)^K \xrightarrow{\alpha} (V/\Lambda)^K \longrightarrow H^1(K, \Lambda/\Lambda_0) \longrightarrow H^1(K, V/\Lambda_0)$$
$$\xrightarrow{\pi} H^1(K, V/\Lambda) \longrightarrow \cdots.$$

The homomorphism α is surjective; indeed, if $x = y + z \in V$ is such that $x - gx = z - gz \in \Lambda$ for all $g \in K$, $x - gx$ is actually in $\Lambda \cap V_K \subset \Lambda_0$. For the same reason, K acts trivially on $\Lambda/\Lambda_0 \simeq \Theta(\Lambda)$. Taking into account (9), we deduce the exact sequence

$$0 \longrightarrow \operatorname{Hom}(K, \Theta(\Lambda)) \longrightarrow H^1(\bar{K}, V_K/\Lambda_K) \oplus \operatorname{Hom}(K, V^K/\Lambda^K)$$
$$\xrightarrow{\pi} H^1(K, V/\Lambda) \longrightarrow \cdots; \tag{10}$$

however, π need not be surjective.

3. Space Groups with Coxeter Point Groups

In this paragraph, we suppose first that K is an essential crystallographic subgroup of Γ generated by reflections. Then K is the Weyl group $W(R)$ of a root system R in V. Our notation follows that of Bourbaki [2]. In particular, we denote by s_α the reflection corresponding to the root α and by $Q(R)$ and $P(R)$ the root and weight lattices of R in V. Since $Q(R)^*$ is easily seen to be $P(R)$, this terminology agrees with that introduced in Section 2. We shall also find it convenient to consider root systems of type A_1 and B_2 as being of type C_1 and C_2, respectively.

Let B be a basis of R. The last root α_m of a component of type C_m in B will be termed *exceptional*. Such roots are distinguished from other elements of B by the fact that the Cartan integer $n(\alpha_m, \beta)$ is even for all $\beta \in B$ or, equivalently, by the fact that $\alpha_m/2$ is a weight.

Let $\tilde{A}(R)$ be the group of those $g \in GL(V)$ which satisfy $g\alpha = a_\alpha h\alpha$ for all $\alpha \in B$, where h is an angle-preserving permutation of B and the a_α are positive real numbers such that

$$n(\beta, \alpha)\, a_\alpha = n(h\beta, h\alpha)\, a_\beta \tag{11}$$

for all $\alpha, \beta \in B$.

PROPOSITION 3.1. *$N(K)$ is the semidirect product of K and $\tilde{A}(R)$.*

Proof. If $g \in N(K)$ and $\alpha \in R$, the conjugate $gs_\alpha g^{-1}$ is a reflection in K and must therefore equal $s_{h\alpha}$ for some $h\alpha \in R$. The equation $gs_\alpha = s_{h\alpha}g$ amounts to saying that

$$\langle x, \check{\alpha}\rangle\, g\alpha = \langle gx, h\check{\alpha}\rangle\, h\alpha \tag{12}$$

for all $x \in V$. Taking $x = \alpha$, we see that $g\alpha = a_\alpha h\alpha$ for some $a_\alpha \in \mathbb{R}$, which can be assumed positive by changing $h\alpha$ to $-h\alpha$ if necessary, and the preceding equation becomes $\langle x, \check{\alpha}\rangle\, a_\alpha = \langle gx, h\check{\alpha}\rangle$. If x is taken to be another root β, we obtain (11). It also follows that for all $\alpha \in R$, $\langle x, \check{\alpha}\rangle > 0$ iff $\langle gx, h\check{\alpha}\rangle > 0$. Consequently, if C is the chamber corresponding to the base B, $g(C)$ is also a chamber whose walls are hyperplanes corresponding to elements of $h(B)$. Therefore $h(B)$ is a basis of R and there exists $g_1 \in K$ such that $g_1(B) = h(B)$. Replacing g by $g_1^{-1}g$ allows us to assume that $h(B) = B$. If we interchange α and β in (11) and multiply the resulting equations, we deduce that $n(\beta, \alpha)\, n(\alpha, \beta) = n(h\beta, h\alpha)\, n(h\alpha, h\beta)$, which implies that α is angle-preserving.

Conversely, suppose that $g \in \tilde{A}(R)$. Then (12) holds if x is a root $\beta \in R$, in view of (11), and therefore holds for all $x \in V$. This means that $gs_\alpha g^{-1} = s_{h\alpha} \in K$ and thus $g \in N(K)$. Finally one notes that the intersection of K with $\tilde{A}(R)$ is trivial since an element $g \neq 1$ in K cannot leave B invariant.

Remark 3.2. When R is irreducible, one sees immediately that $\tilde{A}(R) = H \cdot \tilde{A}_0(R)$, where H is the group of positive homotheties and $\tilde{A}_0(R)$ the group of graph automorphisms of B except in the following cases, when $\tilde{A}_0(R) = \{1, g\}$:

(i) R is of type C_2, $g\alpha_1 = \alpha_2$, $g\alpha_2 = 2\alpha_1$.

(ii) R is of type G_2, $g\alpha_1 = \alpha_2$, $g\alpha_2 = 3\alpha_1$.

(iii) R is of type F_4, $g\alpha_1 = 2\alpha_4$, $g\alpha_2 = 2\alpha_3$, $g\alpha_3 = \alpha_2$, $g\alpha_4 = \alpha_1$.

Indeed, these are the only cases when B admits an angle-preserving permutation which is not a graph automorphism; otherwise, it follows from (11) that $a_\alpha = a_\beta$ whenever $n(\alpha, \beta) \neq 0$. Since B is connected, this means that the a_α's are all equal to a number $a > 0$.

PROPOSITION 3.3. *Every lattice Λ invariant under K is such that $Q(R') \subset \Lambda \subset P(R')$ and $\Lambda^* = P(R')$ for some root system R' satisfying $W(R') = K$.*

Proof. For each $\alpha \in \beta$, let $\Lambda_\alpha = \Lambda \cap \mathbb{R}\alpha$ and $\Lambda_0 = \bigoplus_{\alpha\in\beta} \Lambda_\alpha$. If $x \in \Lambda$, we have $x - s_\alpha(x) = \langle x, \check{\alpha}\rangle\alpha \in \Lambda_0$. This shows that Λ_0 is a lattice since $\langle x, \check{\alpha}\rangle \neq 0$ for some $x \in \Lambda$ and also that $\Lambda_0 \subset \Lambda \subset \Lambda_0{}^*$. Suppose $\Lambda_\alpha = \mathbb{Z}m_\alpha\alpha$ for some $m_\alpha > 0$. Since $m_\alpha\alpha - s_\beta(m_\alpha\alpha) = n(\alpha, \beta)\, m_\alpha\beta$, we must have $n(\alpha, \beta)\, m_\alpha \in \mathbb{Z}m_\beta$ and, similarly, $n(\beta, \alpha)\, m_\beta \in \mathbb{Z}m_\alpha$. This holds if $n(\alpha, \beta) = n(\beta, \alpha) = 0$; on the other hand, it can only happen if

$$\begin{array}{lll} m_\beta = m_\alpha & \text{when} & n(\alpha,\beta) = n(\beta,\alpha) = -1 \\ m_\beta = m_\alpha \ \text{ or } \ m_\beta = 2m_\alpha & \text{when} & n(\alpha,\beta) = -2, \quad n(\beta,\alpha) = -1 \\ m_\beta = m_\alpha \ \text{ or } \ m_\beta = 3m_\alpha & \text{when} & n(\alpha,\beta) = -3, \quad n(\beta,\alpha) = -1. \end{array}$$

Let Π be a component of B and $\Lambda_\Pi = \bigoplus_{\alpha\in\Pi} \Lambda_\alpha$. Using the above equations, one concludes that Λ_Π must be of the form $m_\Pi Q(\Pi')$ for some $m_\Pi > 0$, where $Q(\Pi')$ is the root lattice of a root system with basis Π' and Π' is either equal to Π or to one of the following possibilities:

(i) If $\Pi = \{\alpha_1, ..., \alpha_m\}$ is of type B_m, $\Pi' = \{\alpha_1, ..., \alpha_{m-1}, 2\alpha_m\}$, which is of type C_m.

(ii) If $\Pi = \{\alpha_1, ..., \alpha_m\}$ is of type C_m, $\Pi' = \{2\alpha_1, ..., 2\alpha_{m-1}, \alpha_m\}$, which is of type B_m.

(iii) If $\Pi = \{\alpha_1, ..., \alpha_4\}$ is of type F_4, $\Pi' = \{\alpha_1, \alpha_2, 2\alpha_3, 2\alpha_4\}$, which is also of type F_4.

(iv) If $\Pi = \{\alpha_1, \alpha_2\}$ is of type G_2, $\Pi' = \{3\alpha_1, \alpha_2\}$, which is also of type G_2.

Let R' be the root system with basis B' obtained from B by replacing each component Π with $m_\Pi\Pi'$; we still have $W(R') = K$. However Λ_0 now equals $Q(R')$ and, since $Q(R')^* = P(R')$, we have $Q(R') \subset \Lambda \subset P(R')$. Furthermore, if $x \in \Lambda^*$ and $\alpha \in B'$, then $x - s_\alpha(x) = \langle x, \check{\alpha}\rangle\alpha \in \Lambda_0$ so that $\langle x, \check{\alpha}\rangle \in \mathbb{Z}$ and thus $x \in P(R')$.

If R and R' are root systems of the same type for which $W(R) = W(R') = K$, it is easy to see, using 3.2, that $R' = gR$ for a suitable $g \in \tilde{A}(R)$.

Consequently, lattices Λ satisfying $Q(R) \subset \Lambda \subset P(R)$ are equivalent under $N(K)$ to lattices Λ' satisfying $Q(R') \subset \Lambda' \subset P(R')$. Given K, it therefore suffices to consider only the different *types* of root systems R for which $W(R) = K$. Furthermore, for each type R, one need only consider lattices Λ lying in the range $Q(R) \subset \Lambda \subset P(R)$ *and* satisfying $\Lambda^* = P(R)$. The latter condition is equivalent to

$$\alpha/2 \notin \Lambda \qquad \text{for all} \quad \alpha \in B. \tag{13}$$

Indeed, if $\alpha/2$ belonged to Λ, $\omega_\alpha/2$ would belong to Λ^* (ω_α denotes the fundamental weight corresponding to α), contrary to $\Lambda^* = P(R)$. Conversely, if (13) is satisfied and $x \in \Lambda^*$, we have $\langle x, \check{\alpha}\rangle\alpha \in \Lambda$ and thus $\langle x, \check{\alpha}\rangle \in \mathbb{Z}$ for all $\alpha \in B$ so that $x \in P(R)$.

It is a simple exercise to work out the inequivalent lattices Λ when R is irreducible by looking at the structure of the group $P(R)/Q(R)$ and using 3.2. The results are summarized in Table I.

TABLE I

Type of R	Inequivalent lattices
A_n $(n \geqslant 2)$	$\Lambda_m = \bigcup_{0 \leqslant k \leqslant m} (Q(R) + km'\omega_1)$ where $m \mid n+1$ and $mm' = n+1$.
B_n $(n \geqslant 3)$	$Q(R)$, $P(R)$
C_n	$Q(R)$
D_n (n odd)	$Q(R), Q(R) \cup (Q(R) + 2\omega_n), P(R)$
D_4	$Q(R), Q(R) \cup (Q(R) + \omega_1), P(R)$
D_n (n even and $\geqslant 6$)	$Q(R), Q(R) \cup (Q(R) + \omega_i), P(R)$ where $i = 1, n-1, n$
E_6, E_7	$Q(R)$, $P(R)$
E_8, F_4, G_2	$Q(R)$

We now turn to the calculation of $H^1(K, V/\Lambda)$, *no longer supposing K to be essential.* In accordance with Section 2, we have $V = V^K \oplus V_K$ and $\Lambda \supset \Lambda_0 = \Lambda^K \oplus \Lambda_K$, the projection of Λ on V_K being contained in Λ_K^*. Let R be a root system in V_K for which $W(R)$ equals the restriction of K to V_K and $Q(R) \subset \Lambda_K \subset P(R)$, with $\Lambda_K^* = P(R)$. Suppose $B = \{\alpha_i\}$ is a basis of R and $S = \{s_i\}$ is the set of corresponding generators of K; then $(s_i s_j)^{m_{ij}} = 1$ is a presentation of K, summarized by the Coxeter matrix (m_{ij}). If $\alpha \in B$, we extend the function $\check{\alpha}$ from V_K to V by letting it vanish on V^K.

Let t be a function $S \to V$. According to Section 1, t will induce a cocycle $\bar{t}: K \to V/\Lambda$ iff

$$t((s_i s_j)^{m_{ij}}) = (1 + s_i s_j + \cdots + (s_i s_j)^{m_{ij}-1})(t(s_i) + s_i t(s_j)) \in \Lambda \qquad (14)$$

for all i, j. Suppose $t(s_i) = x_i + \sum_k t_{ki}\alpha_k$, with $x_i \in V^K$ and let $p_{ij} = \langle t(s_i), \check{\alpha}_j \rangle = \sum_k t_{ki} n(k, j)$, where $n(k, j)$ is an abbreviation for $n(\alpha_k, \alpha_j)$. We have $(1 - s_j)\, t(s_i) = p_{ij}\alpha_j$.

PROPOSITION 3.4. (a) *$\bar{t}$ is a coboundary iff $t(s_i) = t_{ii}\alpha_i \bmod \Lambda$.*

(b) $2 \cdot H^1(K, V/\Lambda) = 0$.

Proof. (a) If $a = x + \sum_k a_k\alpha_k \in V$, with $x \in V^K$, the coboundary $K \to V/\Lambda$ corresponding to a $\bmod \Lambda$ maps s_i to $a - s_i a = (\sum_k a_k n(k, i))\, \alpha_i \bmod \Lambda$. Conversely, suppose $t(s_i) = t_{ii}\alpha_i \bmod \Lambda$. The system of equations $\sum_k a_k n(k, i) = t_{ii}$ can be written in the form $\mathbf{aN} = \mathbf{t}$, where $\mathbf{a} = (a_i)$, $\mathbf{t} = (t_{ii})$ and $\mathbf{N}$ is the Cartan matrix of R. Since $\mathbf{N}$ is invertible, the system has a unique solution $\mathbf{a}$ and $\bar{t}$ coincides with the coboundary defined by $a = \sum_k a_k\alpha_k$.

(b) The relation $s_i^2 = 1$ requires that $(1 + s_i)\, t(s_i) \in \Lambda$; it follows that $2t(s_i) = (1 - s_i)\, t(s_i) = p_{ii}\alpha_i \bmod \Lambda$. By (a), this means that $2\bar{t}$ is a coboundary.

By subtracting from t the function $b(s_i) = p_{ii}\alpha_i/2$, which induces a coboundary, we may assume that $p_{ii} \in \mathbb{Z}$.

PROPOSITION 3.5. *The function t induces a cocycle $\bar{t}: K \to V/\Lambda$ iff*

$$2t(s_i) \in \Lambda \qquad \textit{for all } i \qquad (15)$$

$$p_{ij}\alpha_j = p_{ji}\alpha_i \bmod \Lambda \qquad \textit{if} \quad n(i, j) = 0 \qquad (16)$$

$$t(s_i) - t(s_j) = p_{ji}\alpha_j - p_{ij}\alpha_i \bmod \Lambda \qquad \textit{if} \quad n(i, j) = n(j, i) = -1 \quad (17)$$

Proof. Since $s_i^2 = 1$ and $p_{ii} \in \mathbb{Z}$, the relation $(1 + s_i)\, t(s_i) \in \Lambda$ is equivalent to $2t(s_i) \in \Lambda$. If $n(i, j) = 0$, $m_{ij} = 2$; making use of $s_i s_j = s_j s_i$ and the fact that $(1 + s_i)\, t(s_i) \in \Lambda$, (14) can be written as $(1 - s_j)\, t(s_i) = (1 - s_i)\, t(s_j) \bmod \Lambda$, which amounts to (16). If $n(i, j) = n(j, i) = -1$, $m_{ij} = 3$; by a similar manipulation, (14) becomes

$$t(s_i) - t(s_j) = (1 - s_i)(1 - s_j)\, t(s_i) - (1 - s_j)(1 - s_i)\, t(s_j) \bmod \Lambda,$$

which leads to (17). If $n(i,j) = -2$ and $n(j,i) = -1$, $m_{ij} = 4$ and (14) becomes

$$(2 - (1 - s_j)(1 - s_i))(1 - s_j)\, t(s_i)$$
$$= (2 - (1 - s_i)(1 - s_j))(1 - s_i)\, t(s_j) \bmod \Lambda,$$

which is vacuously satisfied since, for example $(1 - s_j)\, t(s_i)$ is a multiple of α_j which is annihilated by $2 - (1 - s_j)(1 - s_i)$. The same situation prevails in the remaining case $n(i,j) = -3$, $n(j,i) = -1$.

COROLLARY 3.6. *A necessary set of conditions for t to induce a cocycle is that*

$$2p_{ij} \in \mathbb{Z} \qquad \text{for all} \quad i, j \tag{18}$$

$$p_{ij} n(j, k) = p_{ji} n(i, k) \bmod \mathbb{Z} \qquad \text{if} \quad n(i,j) = 0 \tag{19}$$

$$p_{ik} - p_{jk} = p_{ji} n(j, k) - p_{ij} n(i, k) \bmod \mathbb{Z} \quad \text{for all } k \text{ if } n(i,j) = n(j,i) = -1 \tag{20}$$

Proof. Since the projection of Λ on V_K is contained in $\Lambda_K{}^* = P(R)$, we can evaluate an element $\check{\alpha}_k$ at both sides of Eqs. (15)–(17) to obtain the above relations.

PROPOSITION 3.7.* *By replacing $\bar{t}$ with a cohomologous cocycle, we may assume that $p_{ij} \in \mathbb{Z}$ except in the following cases (when $i \neq j$):*

(i) *α_i and α_j are exceptional roots and $(\alpha_i - \alpha_j)/2 \in \Lambda$, when* $p_{ij} = p_{ji} \bmod \mathbb{Z}$.

(ii) *α_i is the last and α_j the second last root in a component of type C_m, $m \geqslant 2$, when $\check{\alpha}_j(\Lambda) = \mathbb{Z}$.*

(iii) *α_i and α_j belong to a component of type A_3, B_3 or B_4 and $(\alpha_1 - \alpha_3)/2 \in \Lambda$, when the only exceptions are $p_{13} = p_{31} = p_{23}$* mod $\mathbb{Z}$.

Proof. Suppose $n(i,j) = 0$; in view of (13), Eq. (16) can hold only if $p_{ij} = p_{ji} \bmod \mathbb{Z}$. Furthermore, if $p_{ij} \notin \mathbb{Z}$, $(\alpha_i - \alpha_j)/2$ must be in Λ and also, because of (19), $n(i, k) = n(j, k) \bmod 2\mathbb{Z}$ for all k. If α_i and α_j belong to different components, this is only possible if $n(i, k)$ and $n(j, k)$ are always even, i.e., if α_i and α_j are exceptional. If they belong to the same component Π, there must exist $\alpha_k \in \Pi$ for which $n(i, k) = (n(j, k) = -1$; furthermore, there can be at most one other root $\alpha_{k'} \in \Pi$ and in that case both $n(i, k')$ and $n(j, k')$ must be even. It follows that α_i and α_j can only be the first and third roots, in either order, in a component of a type mentioned in (iii).

Suppose $n(i,j)$ is odd. By adding to t the function defined by $b(s_i) = p_{ij}\alpha_i$ and $b(s_k) = 0$ for $k \neq i$, we can assume that $p_{ij} \in \mathbb{Z}$. It may happen that

* See note added in proof.

$n(i, j')$ is also odd for $j' \neq j$; then $n(j, j')$ is necessarily zero. Applying (20) with $k = j'$, we see that $p_{ij'} - p_{ij} = p_{jj'} \bmod \mathbb{Z}$. The preceding discussion implies that $p_{jj'} \in \mathbb{Z}$ except possibly when α_i is the second root in a component of type A_3 or B_4. In these cases, we can at least assume that $p_{ij} \in \mathbb{Z}$ if $i > j$.

Suppose $n(i, j) = -2$ and $n(j, i) = -1$. If $n(i, j')$ is odd for some j', Eq. (20) with j' replacing j and j replacing k shows that $p_{ij} = p_{j'j} \bmod \mathbb{Z}$. The preceding discussion implies that $p_{j'j} \in \mathbb{Z}$ except possibly when α_i is the second root in a component of type B_3. The only remaining possibility is (ii); if $p_{ij} = \frac{1}{2} \bmod \mathbb{Z}$ in this case Eq. (15) shows that Λ contains an element of the form $\cdots + \omega_j + \cdots$ so that $\check{\alpha}_j(\Lambda) = \mathbb{Z}$.

For the components mentioned in (iii), the proof shows that $p_{13} = p_{31} \bmod \mathbb{Z}$ and that all other $p_{ij} \in \mathbb{Z}$ with the possible exception of p_{23}. Applying (20) with $i = 1$, $j = 2$ and $k = 3$ shows that $p_{23} = p_{13} \bmod \mathbb{Z}$. Finally, (16) implies that if $p_{13} \notin \mathbb{Z}$, $(\alpha_1 - \alpha_3)/2$ must be in Λ.

We shall assume that $p_{ij} \in \mathbb{Z}$ whenever permitted by 3.7.

Since $H^1(K, V/\Lambda)$ is annihilated by 2, it can be considered as a vector space over $\mathbb{Z}/2\mathbb{Z}$. We first compute the dimension $\omega(K, \Lambda)$ of the subgroup $\Omega(K, \Lambda)$ of weightlike classes (see Section 1).

PROPOSITION 3.8. *Let δ be the dimension over $\mathbb{Z}/2\mathbb{Z}$ of the set of elements of order $\leqslant 2$ in $(V^K \oplus P(R))/\Lambda$, ρ the number of connected components in the Dynkin diagram of B after all double and triple bonds have been erased and χ the number of components in B of type C_m. Then $\omega(K, \Lambda) = \delta\rho - \chi$.*

Proof. Since $\Lambda^* = V^K \oplus P(R)$, a cocycle t will be weightlike iff $p_{ij} \in \mathbb{Z}$ for all i, j. According to 3.5, however, a function t with this property will induce a cocycle $\bar{t}$: $K \to V/\Lambda$ (i.e., a homomorphism $K \to \Lambda^*/\Lambda$) iff $2t(s_i) \in \Lambda$ for all i and $t(s_i) = t(s_j) \bmod \Lambda$ whenever $n(i, j) = n(j, i) = -1$. It follows that the dimension of $\mathrm{Hom}(K, \Lambda^*/\Lambda)$ over $\mathbb{Z}/2\mathbb{Z}$ is equal to $\delta\rho$. Since $\Lambda^{**} = V^K \oplus P(R)^*$, the quotient Λ^{**}/Λ^* is isomorphic to $P(R)^*/P(R)$, which in turn is isomorphic to $(\mathbb{Z}/2\mathbb{Z})^\chi$, as can be seen by applying (13) to the irreducible components of R. The assertion now follows from (6).

The number ρ can also be interpreted as the number of conjugacy classes in the set $\{s_i\}$ or as the dimension of $K/[K, K]$ over $\mathbb{Z}/2\mathbb{Z}$.

Remark 3.9. It is easily verified that the only functions of the form $b(s_i) = b_i\alpha_i$ which satisfy the assumption made on p_{ij} are those in which $b_i \in \mathbb{Z}$ unless α_i is an exceptional root, when $2b_i \in \mathbb{Z}$. In any case, the values of b are always weights.

Suppose Π is a component of B of type C_m, where m is odd and $\geqslant 3$. The odd values of m are distinguished from the even by the fact that the weight ω_{m-1} belongs to $Q(R)$. The condition $\check{\alpha}_j(\Lambda) = \mathbb{Z}$ in 3.7(ii) is therefore automatically satisfied. Let t_Π be the function $S \to V$ defined by

$t_\Pi(s_m) = \omega_{m-1}/2$ and $t_\Pi(s) = 0$ if $s \neq s_m$, where s_m is the reflection corresponding to the last root in Π. It is clear from 3.5 that t_Π induces a cocycle. Let $\mathscr{C}$ be the subgroup of $H^1(K, V/\Lambda)$ generated by the cohomology classes of such cocycles.

PROPOSITION 3.10. *The subgroup $\mathscr{C}$ has intersection $\{0\}$ with $\Omega(K, \Lambda)$; its dimension over $\mathbb{Z}/2\mathbb{Z}$ is equal to the number of components in B of type C_m, where m is odd and $\geqslant 3$.*

Proof. Suppose a linear combination $t = \sum_\Pi x_\Pi t_\Pi$, where $x_\Pi \in \mathbb{Z}$, induces a weightlike cocycle. If α_m is the exceptional root in a component Π, the value of $p_{m,m-1}$ for t is equal to $x_\Pi/2$; consequently, x_Π must be even and $\bar{t} = 0$. In view of 3.9, we have also shown that the cohomology classes $\{\bar{t}_\Pi\}$ are independent over $\mathbb{Z}/2\mathbb{Z}$.

In searching for the remaining part of $H^1(K, V/\Lambda)$, we may therefore limit 3.7(ii) to *even* values of m. It happens quite frequently that no further cocycles can exist; for example, this is the case if $\Lambda = \Lambda^K \oplus Q(R)$. More generally, we have the following.

PROPOSITION 3.11.* *Let $\{R^q\}$ be the set of components in R of type C_m, A_3, B_3 or B_4 and R' the remaining part of R. Suppose that*

$$\Lambda = \Lambda^K \oplus \Lambda_K' \oplus \Big(\bigoplus_q \Lambda_K{}^q\Big),$$

where Λ_K' (resp. $\Lambda_K{}^q$) is the intersection of Λ_K with the subspace spanned by the elements of R' (resp. R^q). Then $H^1(K, V/\Lambda) = \Omega(K, \Lambda) \oplus \mathscr{C} \oplus \mathscr{D}$, where the dimension of $\mathscr{D}$ over $\mathbb{Z}/2\mathbb{Z}$ is equal to the number of components R^q of type A_3, B_3 or B_4 for which $\Lambda_K{}^q$ equals $P(R^q)$.

Proof. If α_i and α_j are exceptional roots and $(\alpha_i - \alpha_j)/2 \in \Lambda$, both $\alpha_i/2$ and $\alpha_j/2$ must be in Λ under the hypotheses of the proposition, which contradicts (13); therefore $p_{ij} \in \mathbb{Z}$. Similarly, if α_{m-1} is the second last root in a component of type C_m, m even, the corresponding weight $\omega_{m-1} = \alpha_m/2 \bmod \Lambda$ cannot belong to Λ, so that $\check{\alpha}_{m-1}(\Lambda)$ cannot equal $\mathbb{Z}$. Therefore $p_{m,m-1} \in \mathbb{Z}$. Only case (iii) in 3.7 remains. If $(\alpha_1 - \alpha_3)/2 \in \Lambda$, $\Lambda_K{}^q \neq Q(R^q)$; furthermore, if R^q is of type A_3, $\Lambda_K{}^q$ cannot be the lattice Λ_2 (see Table I) since Eq. (15) would require ω_1 to belong to Λ_2, which it doesn't. Thus $\Lambda_K{}^q$ can only be the lattice $P(R^q)$. However, in this case the function t defined by $t(s_1) = \omega_3/2$, $t(s_2) = \omega_3/2$, $t(s_3) = \omega_1/2$ and, in the case of B_4, $t(s_4) = 0$ does indeed induce a cocycle. The group $\mathscr{D}$ is generated by the cohomology classes of such cocycles; it is not difficult to show, as in the proof of 3.10, that these

* See note added in proof.

classes are independent over $\mathbb{Z}/2\mathbb{Z}$ and that $\mathscr{D}$ has intersection $\{0\}$ with $\Omega(K, \Lambda) \oplus \mathscr{C}$.

For lattices Λ not covered by this proposition one has to determine in each case the further "exceptional" cocycles permitted by 3.7 and 3.5.

From the descriptions of $N(K)$ given earlier, it is possible to examine the effect of $\bar{N}(K, \Lambda)$ on $H^1(K, V/\Lambda)$ in specific cases. For example, suppose K is essential and R is irreducible. If $H^1(K, V/\Lambda)$ is of order 1 or 2 or if the graph of R has no nontrivial automorphisms, the action of $\bar{N}(K, \Lambda)$ is trivial. The only remaining cases are when R is of type D_n, n even, and $\Lambda = Q(R)$. Here $H^1(K, V/\Lambda)$ is of order 4 and there are three orbits if $n \geqslant 6$, but only 2 if $n = 4$.*

4. Application to Classical Crystallography

In the two and three dimensional cases, the results of Section 3 enable one to give a "theoretical" derivation of some of the space groups well known in classical crystallography. We have arranged the results in Tables II and III, using the Schoenflies notation for ease of comparison with [6]. In four of the three-dimensional cases, an additional "exceptional" cocycle is needed to generate $H^1(K, V/\Lambda)$; a list of such cocycles is presented in Table IV.

Finally, in Tables V and VI, we give an interpretation in our terms of the maximal finite subgroups of $GL(n, \mathbb{Z})$ found by Dade [7] in case $n = 4$ and Ryškov [9] in case $n = 5$.

TABLE II

K	Λ	$\Theta(\Lambda)$	Classical	dim $H^1(K, V/\Lambda)$	# orbits
A_2	$Q(R)$		C_{3v}	0	1
	$P(R)$		C_{3s}	0	1
C_2	$Q(R)$		C_{4v}	1	2
G_2	$Q(R)$		C_{6v}	0	1
$C_1 \times C_1$	$Q(R)$		C_{2v}	2	3
	$\{(\alpha_1 + \alpha_2)/2\}$		C_{2k}	0	1
C_1	$Q(R)$	0	C_s	1	2
	$Q(R)$	$P(R)/Q(R)$	C_k	0	1

In the nonessential cases, we have listed Λ_K under Λ; a notation such as $\{\omega\}$ denotes the lattice $Q(R) \cup (Q(R) + \omega)$. The remaining possibilities for K are the rotation subgroups of the groups listed above.

* See note added in proof.

TABLE III

K	Λ	$\Theta(\Lambda)$	Classical	dim $H^1(K, V/\Lambda)$	# orbits
A_3	$Q(R)$		$T_{d\beta}$	1	2
	A_2		$T_{d\alpha}$	1	2
	$P(R)$		$T_{d\gamma}$	1	2
B_3	$Q(R)$		$O_{h\alpha}$	2	4
	$P(R)$		$O_{h\gamma}$	1	2
C_3	$Q(R)$		$O_{h\beta}$	2	4
$C_1 \times A_2$	$Q(R)$		$D_{3h\delta}$	1	2
	$Q(C_1) \oplus P(A_2)$		$D_{3h\epsilon}$	1	2
$C_1 \times C_2$	$Q(R)$		$D_{4h\alpha}$	4	16
	$\{(\alpha_1+\alpha_3)/2\}$		$D_{4h\beta}$	2*	4
$C_1 \times G_2$	$Q(R)$		D_{6h}	2	4
$C_1 \times C_1 \times C_1$	$Q(R)$		$D_{2h\alpha}$	6	16
	$\{(\alpha_1+\alpha_2+\alpha_3)/2\}$		$D_{2h\gamma}$	3	4
	$\{(\alpha_1+\alpha_2)/2\}$		$D_{2h\delta}$	3	6
	$\{(\alpha_1+\alpha_2)/2, (\alpha_1+\alpha_3)/2, (\alpha_2+\alpha_3)/2\}$		$D_{2h\beta}$	1*	2
A_2	$Q(R)$	0	$C_{3v\delta}$	1	2
	$Q(R)$	$P(R)/Q(R)$	$C_{3v\alpha}$	1	2
	$P(R)$	0	$C_{3v\epsilon}$	1	2
C_2	$Q(R)$	0	$C_{4v\alpha}$	3	8
	$Q(R)$	$P(R)/Q(R)$	$C_{4v\beta}$	2*	4
G_2	$Q(R)$	0	C_{6v}	2	4
$C_1 \times C_1$	$Q(R)$	0	$C_{2v\alpha}$	4	10
	$Q(R)$	$\{0, (\alpha_1+\alpha_2)/2\}$	$C_{2v\gamma}$	2	3
	$Q(R)$	$\{0, \alpha_1/2\}$	$C_{2v\epsilon}$	2	4
	$\{(\alpha_1+\alpha_2)/2\}$	0	$C_{2v\delta}$	2	3
	$\{(\alpha_1+\alpha_2)/2\}$	$\{0, \alpha_1/2\}$	$C_{2v\beta}$	1*	2
C_1	$Q(R)$	0	$C_{s\alpha}$	2	2
	$Q(R)$	$P(R)/Q(R)$	$C_{s\beta}$	1	2
$\pm A_2$	as for A_2		$D_{3d\alpha}$	1	2
			$D_{3d\delta}$	1	2
			$D_{3d\epsilon}$	1	2
$\pm C_1$	as for C_1		$C_{2h\alpha}$	3	4
			$C_{2h\beta}$	1	2

The presence of an "exceptional" cocycle is indicated by *. The remaining possibilities for K are the rotation subgroups of the 11 Coxeter groups in the above table, five groups obtained by adding -1 to rotation subgroups and three exceptional groups, whose Schoenflies names are S_4, D_{2d} and C_{3h}.

TABLE IV

K	cocycle
$C_1 \times C_2$	$t(s_1) = \omega_3/2$, $t(s_2) = 0$, $t(s_3) = (\omega_1 + \omega_2)/2$
$C_1 \times C_1 \times C_1$	$t(s_1) = (\omega_2 + \omega_3)/2$, $t(s_2) = (\omega_1 + \omega_3)/2$, $t(s_3) = (\omega_1 + \omega_2)/2$
C_2	$t(s_1) = 0$, $t(s_2) = \frac{1}{2}(a/2 + \omega_1)$, where $a/2 + \omega_1 \in \Lambda$, $a \in \Lambda^K$
$C_1 \times C_1$	$t(s_1) = \frac{1}{2}(a/2 + \omega_2)$, $t(s_2) = \frac{1}{2}(a/2 + \omega_1)$

TABLE V

K	Λ	Dade	order of K
$\pm A_4$	$Q(R)$	Sx_4	240
	$P(R)$	Py_4	240
B_4	$Q(R)$	Cu_4	192
F_4	$Q(R)$	Qn	1152
$C_2 \times G_2$	$Q(R)$	$Sx_2 \otimes Cu_2$	96
$C_1 \times B_3$	$Q(C_1) \oplus P(B_3)$	$Py_3 \otimes Cu_1$	96
$C_1 \times C_3$	$Q(R)$	$Sx_3 \otimes Cu_1$	96
$A(G_2 \times G_2)$	$Q(R)$	$Sx_2^{(2)}$	288
T	$Q(R) \otimes Q(R)$ R of type A_2	$Sx_2^{\otimes 2}$	144

The group $A(G_2 \times G_2)$ is the complete group of automorphisms of a root system of type $G_2 \times G_2$. The last group $T = Sx_2^{\otimes 2}$ does not seem to be of Coxeter type; it is the group of automorphisms of the quadratic form

$$2x_1^2 + 2x_2^2 + 2x_3^2 + 2x_4^2 - 2x_1x_2 - 2x_1x_3 + x_1x_4 + x_2x_3 - 2x_2x_4 - 2x_3x_4 .$$

TABLE VI

K	Λ	order of K
$\pm A_5$	$Q(R)$, A_2, A_3 or $P(R)$	1440
B_5	$Q(R)$ or $P(R)$	3840
C_5	$Q(R)$	3840
$G_2 \times B_3$	$Q(R)$ or $P(R)$	596
$G_2 \times C_3$	$Q(R)$	596
$C_2 \times B_3$	$Q(C_2) \oplus P(B_3)$	384
$C_2 \times C_3$	$Q(R)$	384
$C_1 \times F_4$	$Q(R)$	2304
$C_1 \times (\pm A_4)$	$Q(R)$ or $Q(C_1) \oplus P(A_4)$	480
$C_1 \times A(G_2 \times G_2)$	$Q(R)$	576
$C_1 \times T$	$Q(C_1) \oplus (Q(R) \otimes Q(R))$ (R of type A_2)	288

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Note Added in Proof. We have neglected the case of D_4 in several places. In Proposition 3.7, one should include it under (iii). The exceptional cases can then be $p_{13} = p_{31} = p_{23}$, $p_{14} = p_{41} = p_{24}$, and $p_{34} = p_{43} = p_{23} + p_{24}$; correspondingly, the elements $(\alpha_1 - \alpha_3)/2$, $(\alpha_1 - \alpha_4)/2$, and $(\alpha_3 - \alpha_4)/2$ must belong to Λ. In Proposition 3.11, it should also be included among the components $\{R^q\}$. Since precisely one of the exceptions cannot occur, $\Lambda_K{}^q$ must again be the lattice $P(R^q)$. The two cocycles $t(s_1) = t(s_2) = t(s_4) = \omega_3/2$, $t(s_3) = \omega_1/2 + \omega_4/2$ and $t'(s_1) = t'(s_2) = t'(s_3) = \omega_4/2$, $t'(s_4) = \omega_1/2 + \omega_3/2$ then generate a summand of type $\mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}$ in $\mathscr{D}$, so that one has to add to its dimension *twice* the number of components R^q of type D_4 for which $\Lambda_K{}^q$ equals $P(R^q)$. Finally, in the last paragraph of Section 3, $H^1(K, V/\Lambda)$ is also of order 4 if K is of type D_4 and $\Lambda = P(R)$, but there are still only 2 orbits.

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